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ROMBERG INTEGRATION

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SUMMARY

This paper presents a theoretical development of a procedure to numerically integrate the definite integral $\int_a^b f(t)\,dt$. Theorems and the majority of proofs are given, justifying the procedure, and remarks are made concerning the types of functions for which the procedure appears well suited.

INTRODUCTION

This report presents a theoretical method to numerically integrate the definite integral $\int_a^b f(t)\,dt$. A special case of the method, the Romberg Integration scheme, is also presented. Theorems and the majority of proofs are given justifying the procedure, and remarks are made concerning types of functions for which the procedure appears well suited. Emphasis has been placed on the mathematical justification of the procedure in order to provide a deeper understanding of the method, and, hopefully, to lead to further research of the procedure and its modifications.

The chief references from which the bulk of the material of this paper was obtained are Moler[1] and Bauer, Rutishauser, and Stiefel.[2]

The author wishes to thank Mr. Robert Meyers for the many helpful suggestions made during the preparation of this paper.

SYMBOLS

P_{2n}, $n = 1,2,\cdots$	Bernoulli numbers
E_m, $m = 0,1,\cdots$	real constants
f_n, $n = 0,1,\cdots$	$f(a + n\,h)$
$f^{(n)}$, $n = 1,2,\cdots$	n^{th} derivative of f
h	integration step-size
h_k	$(b - a)/N_k$
$M(h)$	midpoint rule sum
N_k, $k = 0,1,\cdots$	increasing sequence of positive integers
$P_j^{(k)}(x)$	$(k-j)^{th}$ degree polynomial interpolating the points (x_i, y_i), $i = j,\cdots,k$
$p_j^{(k)}$	value at x^* of $P_j^{(k)}(x)$

$Q_{j,s}^{(k)}$	value at 0 of the polynomial which interpolates the function x^s ; ($s \geq 1$, at the points x_i , $i = j,\cdots,k$)
$T(0)$	$\int_a^b f(t)\, dt$
$T(h)$	trapezoidal sum
$T_j^{(k)}$	value at 0 of $P_j^{(k)}(x)$
x_i, $i = 0,1,\cdots$	distinct real or complex numbers
y_i, $i = 0,1,\cdots$	real or complex numbers not necessarily distinct
σ, ρ	constants between 0 and 1

NEVILLE'S ALGORITHM

Suppose that we are given (m+1) distinct points, $x_0, x_1, \cdots, x_m$, real or complex, and (m+1) corresponding values (not necessarily distinct), $y_0, y_1, \cdots, y_m$. Neville's algorithm is a method of calculating the unique polynomial $P(x)$ of degree m which takes on the values y_k at the points x_k.

To describe the method, let $P_j^{(k)}(x)$ denote the interpolating polynomial of degree (k-j) which satisfies $P_j^{(k)}(x_i) = y_i$, $(i = j,\cdots,k)$.

(1.1) THEOREM. For $j = k$, let $P_k^{(k)}(x) = y_k$ and for $j < k$, let

$$P_j^{(k)}(x) = \left[(x_k - x)\, P_j^{(k-1)}(x) - (x_j - x)\, P_{j+1}^{(k)}(x)\right] \Big/ (x_k - x_j) \tag{1.2}$$

$P_j^{(k)}(x)$ is then the unique polynomial of degree (k-j), which interpolates the points $(x_j, y_j), \cdots, (x_k, y_k)$.

Proof. Induction is used on $n = k - j$. If $n = 0$, the theorem is obvious. Suppose the theorem has been proved

for $n = m$. Then

$$P_j^{(j+m+1)}(x) = \Big[(x_{j+m+1} - x)\, P_j^{(j+m)}(x)$$

$$- (x_j - x)\, P_{j+1}^{(j+m+1)}(x)\Big] \Big/ (x_{j+m+1} - x_j)$$

and by the induction hypothesis, $P_j^{(j+m)}(x)$ and $P_{j+1}^{(j+m+1)}(x)$ are polynomials of degree m , and hence $P_j^{(j+m+1)}(x)$ is a polynomial of degree $m+1$. Further, by direct verification, $P_j^{(j+m+1)}(x_i) = y_i$ for $i = j, j+m+1$. By assumption, for $j < i < j+m+1$, $P_j^{(j+m)}(x_i) = P_{j+1}^{(j+m+1)}(x_i) = y_i$; hence $P_j^{(j+m+1)}(x_i) = y_i$ for $j < i < j+m+1$.

Finally, the uniqueness follows from the fact that if $P(x)$ and $Q(x)$ are two polynomials of degree n interpolating the same $(n+1)$ distinct points, then $P(x) - Q(x)$ is a polynomial of degree n having at least $(n+1)$ roots and thus is the zero polynomial. Therefore $P(x) = Q(x)$.

Neville's algorithm then can be used to evaluate the interpolating polynomial $P_j^{(k)}(x)$ at any desired point x^* . An important advantage of Neville's algorithm over the, perhaps, more familiar Lagrangian representation is that the number of points to be interpolated may be increased without redoing previous computation. For example, if we wish to

calculate $P_0^{(4)}(x)$, then it is only necessary to calculate $P_0^{(3)}(x)$ and $P_1^{(4)}(x)$ and apply (1.2) to compute $P_0^{(4)}(x)$. Thus, the 4^{th} degree interpolating polynomial $P_0^{(4)}(x)$ is determined by using linear interpolation on $\left(x_0, P_0^{(3)}(x)\right)$ and $\left(x_4, P_1^{(4)}(x)\right)$. That this is true in general is clear. It is also important to realize that no assumption has been made regarding the distribution of the points x_k . They need neither be equally spaced, nor in increasing or decreasing order.

If we use the notation $P_j^{(k)}$ for the computed values $P_j^{(k)}(x^*)$, then Neville's algorithm can be arranged in the following table:

$$\begin{array}{ccccc}
P_0^{(0)} & & & & \\
P_1^{(1)} & P_0^{(1)} & & & \\
P_2^{(2)} & P_1^{(2)} & P_0^{(2)} & & \\
P_3^{(3)} & P_2^{(3)} & P_1^{(3)} & P_0^{(3)} & \\
\vdots & \vdots & \vdots & \vdots & \ddots \\
P_k^{(k)} & P_{k-1}^{(k)} & P_{k-2}^{(k)} & P_{k-3}^{(k)} & P_0^{(k)} \\
\vdots & \vdots & \vdots & \vdots & \vdots
\end{array} \tag{1.3}$$

Using this arrangement each entry $P_j^{(k)}$ is obtained directly from the two entries $P_j^{(k-1)}$ and $P_{j+1}^{(k)}$ immediately to the "left" and "left-above" it.

In the usual case, $T(x)$ is a function such that $T(x_i) = y_i$ for $0 \leq i \leq n$. To approximate $T(x^*)$ by using polynomial interpolation, we iteratively compute the values $P_j^{(k)}$ until two or more successive values, $P_0^{(k)}$, $P_0^{(k+1)}$, $\cdots$, agree to within some preassigned degree of accuracy.

Finally, we note that if $x^* = 0$,

$$P_j^{(k)} = \left[x_k P_j^{(k-1)} - x_j P_{j+1}^{(k)}\right] / (x_k - x_j) \qquad (1.4)$$

We shall be interested in this form when using the Romberg scheme.

ROMBERG INTEGRATION

One of the most well-known methods of approximating the integral $\int_a^b f(t)\,dt$ is the trapezoid rule. If N is a positive integer and

$$h = (b - a)/N$$

$$x_n = a + nh$$

$$f_n = f(x_n) \ , \quad n = 0,1,2,\cdots,N$$

then the N-interval trapezoid rule determined by the N-subintervals, (x_i, x_{i+1}), $i = 0,1,\cdots,N-1$, is given by

$$T(h) = h\left(\frac{1}{2} f_0 + f_1 + \cdots + f_{N-1} + \frac{1}{2} f_N\right) \tag{2.1}$$

where h is the mesh size.

It follows easily, then, that if $\int_a^b f(t)\,dt$ exists, $T(h) \to \int_a^b f(t)\,dt$ as $h \to 0$. Further, if $f''(t)$ is continuous on $[a,b]$, and hence bounded on $[a,b]$, then

$$T(h) = \int_a^b f(t)\,dt + [(b - a)\,h^2/12] \cdot f''(\xi)$$

where $\xi \in (a,b)$.

The Romberg method consists of an application of Neville's algorithm to the function $T(h)$. In general, let $N_0, N_1, \cdots, N_k, \cdots$ be an increasing sequence of positive integers and

$$
\begin{aligned}
h_k &= (b - a)/N_k \\
x_k &= h_k^2 \\
y_k &= T(h_k) \ , \quad k = 0,1,\cdots
\end{aligned}
\tag{2.2}
$$

Applying Neville's algorithm with $x^* = 0$ and $T_j^{(k)}$ denoting the value $P_j^{(k)}$, we have from (1.4),

For $j = k$, $T_k^{(k)} = T(h_k)$ and for $j < k$,

$$T_j^{(k)} = \left[h_k^2 \, T_j^{(k-1)} - h_j^2 \, T_{j+1}^{(k)}\right] \Big/ \left(h_k^2 - h_j^2\right) \tag{2.3}$$

Thus, $T_j^{(k)}$ is the value at 0 of the $(k-j)^{th}$ degree polynomial which interpolates the $(k-j+1)$ points, $\left(h_j^2, T(h_j)\right)$, $\cdots$, $\left(h_k^2, T(h_k)\right)$. Therefore, from (1.3) we have the following table:

$$
\begin{array}{lllll}
T_0^{(0)} & & & & \\
T_1^{(1)} & T_0^{(1)} & & & \\
T_2^{(2)} & T_1^{(2)} & T_0^{(2)} & & \\
T_3^{(3)} & T_2^{(3)} & T_1^{(3)} & T_0^{(3)} & \\
\vdots & \vdots & \vdots & \vdots & \ddots \\
T_k^{(k)} & T_{k-1}^{(k)} & T_{k-2}^{(k)} & T_{k-3}^{(k)} & T_0^{(k)} \\
\vdots & \vdots & \vdots & \vdots & \vdots
\end{array}
\tag{2.4}
$$

Each entry in the table is an approximation to $T(0)$; that is, $\int_a^b f(t)\,dt$. The first column (which we shall call the zeroth column) contains the values of the successive trapezoid rules. We should note here that the process just described is often called Romberg Integration. However, we shall restrict ourselves to this terminology for only the special case $N_k = 2^k$. The general procedure just described will be referred to as a modification or generalization of the Romberg scheme. As we shall see in Section III, the basis for this procedure will be the existence of an asymptotic expansion of $T(h)$ in powers of h^2 . For this

reason, the above process is often referred to as extrapolation to the limit or Richardson's deferred approach to the limit.[3]

As noted previously, the Romberg scheme uses the values $N_k = 2^k$, $k = 0,1,\cdots$. This choice has several advantages for computational purposes. For $h = (b - a)/N$, let $M(h)$ be the N-interval midpoint rule; that is

$$M(h) = h \sum_{n=1}^{N} f\left(a + \left(n - \tfrac{1}{2}\right) h\right)$$

Since

$$T(h) = h\left[\sum_{n=1}^{N-1} f(a + n\,h) + (1/2)\left(f(a) + f(b)\right)\right]$$

it follows that $T(h/2) = (T(h) + M(h))/2$. For the Romberg scheme, since $h_{k+1} = h_k/2$, it follows that

$$T(h_{k+1}) = \left(T(h_k) + M(h_k)\right)\Big/2 \qquad (2.5)$$

This relation was used by Romberg to construct the zeroth column of his array. Furthermore, using the fact that $h_j/h_k = 2^{k-j}$, (2.3) can be written in the form:

$$T_j^{(k)} = T_{j+1}^{(k)} + \left(T_{j+1}^{(k)} - T_j^{(k-1)}\right)\Big/(4^{k-j} - 1) \qquad (2.6)$$

In this form, the algorithm was first described by Romberg and is called Romberg Integration.[4]

However, while the choice $N_k = 2^k$ has many "nice" computational features, it also has the disadvantage that the number of grid points at which f must be evaluated doubles with each iteration. If f is a complicated function, this could be a significant disadvantage.

The natural suggestion would be to choose a sequence N_k less rapidly increasing than the sequence $\left\{2^k\right\}_{k=0}^{\infty}$. However, before we consider such chcices, we should concern ourselves with the question of when does the Romberg scheme converge to $\int_a^b f(t)\, dt$. We shall consider this problem and others in the next section.

CONVERGENCE CRITERIA

Our first aim in this section will be to justify the Romberg scheme. We will show that every diagonal and every column of (2.4) with $N_k = 2^k$ $(k = 0,1,\cdots)$ converges to $T(0)$. Proofs are based on those in ref. 2.

It is clear that every entry of (2.4) is a linear combination of elements of the zeroth column; that is,

$$T_k^{(k+m)} = \sum_{i=0}^{m} c_{m,m-i}\, T_{k+i}^{(k+i)} \tag{3.1}$$

where the coefficients $c_{m,m-i}$ are independent of k . From (2.6), it follows that for $m \neq 0$,

$$T_k^{(k+m)} = \left(4^m\, T_{k+1}^{(k+m)} - T_k^{(k+m-1)}\right)\Big/(4^m - 1) \tag{3.2}$$

From this observation and from (3.1), it follows easily by induction on m that for $m \neq 0$, the coefficients $c_{m,m-i}$ obey the recursion formula

$$c_{m,m-i} = \left[4^m\, c_{m-1,m-i} - c_{m-1,m-1-i}\right]\Big/(4^m - 1) \tag{3.3}$$

for $i = 0,1,\cdots,m$, assuming $c_{m-1,m} = c_{m-1,-1} = 0$.

If $t_m(x)$ are the polynomials defined by

$$t_m(x) = \sum_{k=0}^{m} c_{m,k}\, x^k \, , \quad m = 0,1,2,\cdots \tag{3.4}$$

then from (3.3) we have that, for $m \neq 0$,

$$t_m(x) = \sum_{k=0}^{m} \left[\left(4^m c_{m-1,k} - c_{m-1,k-1}\right) \Big/ (4^m - 1) \right] x^k$$

$$= \left[(4^m - x)/(4^m - 1) \right] \sum_{k=0}^{m-1} c_{m-1,k}\, x^k$$

$$= (4^m - x)\, t_{m-1}(x)/(4^m - 1)$$

From this result it follows that, for $m \neq 0$,

$$t_m(x) = \left[\Pi_{i=1}^{m} (4^i - x) \right] \Big/ \left[\Pi_{i=1}^{m} (4^i - 1) \right] \tag{3.5}$$

which, together with the fact that $c_{0,0} = 1$, allows us to conclude that

$$t_m(1) = \sum_{i=0}^{m} c_{m,i} = \sum_{i=0}^{m} c_{m,m-i} = 1 \tag{3.6}$$

for each m .

Further, we have the following:

(3.7) LEMMA. For each m, $\sum_{i=0}^{m} |c_{m,i}| < 2$

Proof.— Since

$$t_m(-1) = \left[\Pi_{i=1}^{m}(4^i + 1)\right] \Big/ \left[\Pi_{i=1}^{m}(4^i - 1)\right]$$

$$\leq \left[\Pi_{i=1}^{\infty}(4^i + 1)/(4^i - 1)\right] < 2$$

it suffices to show that $\sum_{i=0}^{m} |c_{m,i}| = t_m(-1)$ for each m. To prove this, it is sufficient to show that $(-1)^i c_{m,i} > 0$ for $i = 0,1,2,\cdots,m$. Suppose that $m = 1$. Since $(-1)^0 c_{m,0} = c_{m,0} = t_m(0) > 0$ for all m, we have that $(-1)^0 c_{1,0} > 0$. Further, using (3.1) and (3.2), it can be observed that $c_{1,1} = -1/3$; hence $(-1)^1 c_{1,1} = 1/3 > 0$. Suppose the statement has been proved for $m = n - 1$. We consider $(-1)^i c_{n,i}$, where $i \in \{0,1,\cdots,n-1\}$. From (3.3),

$$(-1)^i c_{n,i} = \left[4^n(-1)^i c_{n-1,i} - (-1)^i c_{n-1,i-1}\right] \Big/ (4^n - 1)$$

and by the induction hypothesis, $(-1)^i c_{n-1,i} > 0$, and $(-1)^{i-1} c_{n-1,i-1} > 0$ for $i \in \{0,1,\cdots,n-1\}$. Therefore,

$\left[4^n(-1)^i\, c_{n-1,i} + (-1)^{i-1}\, c_{n-1,i-1}\right] \Big/ (4^n - 1) > 0$. Finally,

$$(-1)^n\, c_{n,n} = \left[4^n(-1)^n\, c_{n-1,n} - (-1)^n\, c_{n-1,n-1}\right] \Big/ (4^n - 1)$$

$$= \left[0 + (-1)^{n-1}\, c_{n-1,n-1}\right] \Big/ (4^n - 1) > 0$$

since $(-1)^{n-1}\, c_{n-1,n-1} > 0$ by the induction hypothesis.

Before the convergence of the Romberg method can be shown, we need to observe that for each k ,

$$\lim_{m\to\infty} c_{m,m-k} = 0 \tag{3.8}$$

To show this, observe that from (3.5)

$$t_m(4x) = 4^m\, t_m(x)(1 - x)/(4^m - x)$$

and

$$t_{m-1}(x) = t_m(x)(4^m - 1)/(4^m - x)$$

Hence

$$t_m(4x) - t_m(x) = -x\, t_{m-1}(x)$$

or

$$\sum_{k=0}^{m} c_{m,k}(4^k - 1)\, x^k = -\sum_{k=0}^{m-1} c_{m-1,k}\, x^{k+1}$$

By equating coefficients, we then have

$$c_{m,k} = -c_{m-1,k-1}/(4^k - 1)$$

Repeated application of this last relation gives

$$c_{m,m-k} = (-1)^{m-k} c_{k,0} \Big/ \Pi_{i=1}^{m-k} (4^i - 1) \tag{3.9}$$

From this last relation, (3.8) is apparent.

The convergence of the Romberg scheme may now be proved.

(3.10) THEOREM. The convergence of the zeroth column of the array (2.4) implies the convergence of all further columns of (2.4) to the same limit.

Proof. Suppose that $\lim_{k\to\infty} T_k^{(k)} = T(0) = \int_a^b f(t)\,dt$. Consider the elements $T_k^{(k+m)}$, $k = 0,1,\cdots$, of the m^{th} column, where $T_k^{(k+m)} = \sum_{i=0}^m c_{m,m-i} T_{k+i}^{(k+i)}$ for each k . We show that $\lim_{k\to\infty} T_k^{(k+m)} = T(0)$. Let $\varepsilon > 0$ be assigned. Choose N , a positive integer, such that $\left|T_k^{(k)} - T(0)\right| < \varepsilon/[(m + 1)\, U]$ for $k \geq N$, where $U = \max \left|c_{m,m-i}\right|$, $i = 0,\cdots,m$. By (3.6) $\sum_{i=0}^m c_{m,m-i} = 1$;

hence

$$T_k^{(k+m)} - T(0) = \sum_{i=0}^{m} c_{m,m-i}\, T_{k+i}^{(k+i)} - T(0)$$

$$= \sum_{i=0}^{m} c_{m,m-i}\, T_{k+i}^{(k+i)} - \sum_{i=0}^{m} c_{m,m-i}\, T(0)$$

$$= \sum_{i=0}^{m} c_{m,m-i}\left(T_{k+i}^{(k+i)} - T(0)\right)$$

Therefore, for $k \geq N$,

$$\left|T_k^{(k+m)} - T(0)\right| < (m+1)\, U \cdot \varepsilon/[(m+1) \cdot U] = \varepsilon$$

and the theorem is proved.

(3.11) THEOREM. The convergence of the zeroth column of the array (2.4) implies the convergence of all diagonal sequences; that is, of all sequences $T_k^{(k+m)}$, k constant, $m \to \infty$, to the same limit.

Proof. Let k be a fixed nonnegative integer. Under the assumption that $\lim_{k\to\infty} T_k^{(k)} = T(0) = \int_a^b f(t)\,dt$, we show that $\lim_{m\to\infty} T_k^{(k+m)} = T(0)$. We note that a sequence-to-sequence transformation is established by (3.1) between the

sequences $\left\{T_{k+i}^{(k+i)}\right\}_{i=0}^{\infty}$ and $\left\{T_k^{(k+m)}\right\}_{m=0}^{\infty}$. Then, according to the Silverman-Toeplitz theorem (Theorem 4.1, II, p. 64),[5] a necessary and sufficient condition that $T_k^{(k+m)} \to T(0)$, as $m \to \infty$, is that

(a) $\sum_{i=0}^{m} |c_{m,m-i}| \leq M$ for every positive integer $m \geq N_0$,

(b) $\lim_{m\to\infty} c_{m,m-k} = 0$ for each fixed k, and

(c) $\sum_{i=0}^{m} c_{m,m-i} = A_m \to 1$, as $m \to \infty$.

These conditions are satisfied by Theorem (3.7) and statements (3.6) and (3.8).

Thus, under only the assumption that f is Riemann integrable on $[a,b]$, the convergence of the Romberg scheme has been shown. Therefore, in the usual case of interest, noted in Section I, the diagonal entries $T_0^{(k)}$ converge to $T(0)$ if only $\int_a^b f(t)\,dt$ exists. However, it has not yet been shown which column or diagonal converges to $T(0)$ "faster." The remainder of this section will be concerned with this problem.

(3.12) Definition. A function $f(x)$ has "order x^k as x approaches 0," and we write $f(x) = O(x^k)$, if constants M and x_0 exist such that for all $|x| \leq x_0$, $|f(x)| \leq M|x^k|$.

(3.13) Definition. A function $f(x)$ has an asymptotic series as x approaches 0, if constants $a_0, a_1, \cdots$ exist such that for all m

$$y(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m + O(x^{m+1}) \qquad (3.14)$$

(3.15) THEOREM. If $f^{(2m+2)}(t)$ is continuous for $a \leq t \leq b$, then there are numbers $a_1, \cdots, a_m$ depending on f, but not on h, so that

$$T(h) = \int_a^b f(t)\,dt + a_1 h^2 + \cdots + a_m h^{2m} + O(h^{2m+2}) \qquad (3.16)$$

In other words, $T(h)$ as an expansion consisting of the first $(m+1)$ terms of an asymptotic series.

Proofs of this result will be found in Ralston[6] and Henrici (Theorem 13.6, p. 257).[7] We can now prove a theorem which is of a more general nature than the Romberg scheme and which will describe the "speed of convergence" of the columns of the array (1.3). We will consider the quantities $P_j^{(k)}$

as j and k both tend to infinity, with $n = k - j$ held fixed. These form the n^{th} column of the array (1.3), continuing to designate the first column as the zeroth column. The theorem and the proof given here are in ref. 1. It is essentially the same theorem as that given in ref. 7 (Theorem 12.4, p. 240), except that in the latter theorem, it is assumed that the ratio $(h_{k+1}/h_k)^2$ is a fixed constant between 0 and 1 for all k.

(3.17) THEOREM. Assume that for m, a positive integer, the function $y(x)$ has an expansion consisting of the first $m+1$ terms of an asymptotic series; that is,

$$y(x) = a_0 + a_1 x + \cdots + a_m x^m + O(x^{m+1}) \qquad (3.18)$$

as x approaches 0. Assume further that the evaluation points $x_0, x_1, \cdots$ satisfy

$$0 < \sigma \leq x_k / x_{k-1} \leq \rho < 1 \qquad (3.19)$$

for all k. Then, for $n < m$, the values $P_{k-n}^{(k)}$ defined by $P_{k-n}^{(k)} = P_{k-n}^{(k)}(0)$ with $j = k - n$ satisfy

$$P_{k-n}^{(k)} = a_0 + (-1)^n a_{n+1} x_{k-n} \cdots x_k + O\left(x_k^{n+2}\right) \qquad (3.20)$$

as k approaches ∞. Furthermore, if $a_n \neq 0$, then

$$\lim_{k\to\infty}\left(\left[P_{k-n}^{(k)} - a_0\right] \Big/ \left[P_{k-n+1}^{(k)} - a_0\right]\right) = 0 \qquad (3.21)$$

That is, the n^{th} column converges to a_0 faster than the $(n-1)^{st}$ column.

Moler[1] proves the theorem by first proving the following lemma.

(3.22) LEMMA. Assume $x_0, x_1, \cdots$ satisfy (3.19) and for any positive integer s define $Q_{j,s}^{(k)}$ by

$$Q_{k,s}^{(k)} = x_k^s$$

and for $j < k$,

$$Q_{j,s}^{(k)} = \left[x_k\, Q_{j,s}^{(k-1)} - x_j\, Q_{j+1,s}^{(k)}\right] \Big/ [x_k - x_j]$$

Then

$$Q_{k-n,s}^{(k)} = \begin{cases} 0 & \text{, if } s \le n & (3.23) \\ (-1)^n\, x_{k-n} \cdots x_k, & \text{if } s = n+1 & (3.24) \\ O\left(x_k^s\right) \text{ as } k \to \infty & \text{, if } s \ge n+2 & (3.25) \end{cases}$$

Proof. By Theorem (1.1) $Q^{(k)}_{k-n,s}$ is the value at 0 of the polynomial of degree n which interpolates the function x^s at the points $x_{k-n}, \cdots, x_k$.

Case 1. $s \leq n$. $Q^{(k)}_{k-n,s}(x) - x^s$ is a polynomial of degree n, which has $n+1$ zeros. Hence, it is identically zero and therefore $Q^{(k)}_{k-n,s} = 0$. (In fact, $s = n$.)

Case 2. $s = n + 1$. $Q^{(k)}_{k-n,s}(x) - x^{n+1}$ is a polynomial of degree $n+1$, which has the $n+1$ roots, $x_{k-n}, \cdots, x_k$. Thus, by the fundamental theorem of algebra,

$$Q^{(k)}_{k-n,s}(x) - x^{n+1} = -1(x - x_{k-n}) \cdots (x - x_k)$$

Therefore,

$$Q^{(k)}_{k-n,s} = -1(-1)^{n+1} x_{k-n} \cdots x_k = (-1)^n x_{k-n} \cdots x_k$$

Case 3. $s \geq n + 2$. We use (3.19) and induction on n. Let $n = 0$. Then $Q^{(k)}_{k,s} = x^s_k = O\left(x^s_k\right)$. Assume the statement has been proved for $n = m - 1$. Then

$$Q^{(k)}_{k-m,s} = \left[x_k \, Q^{(k-1)}_{k-m,s} - x_{k-m} \, Q^{(k)}_{k-m+1,s}\right] \Big/ (x_k - x_{k-m})$$

By the induction hypothesis, we have

$$Q_{k-m,s}^{(k)} = \left[x_k\, O\left(x_{k-1}^s\right) - x_{k-m}\, O\left(x_k^s\right)\right] \Big/ (x_k - x_{k-m})$$

$$= \left[(x_k/x_{k-m})\, O\left(x_{k-1}^s\right) - O\left(x_k^s\right)\right] \Big/ \left((x_k/x_{k-m}) - 1\right)$$

Since $0 < \sigma \le x_k/x_{k-1}$, $O\left(x_{k-1}^s\right) = O\left(x_k^s\right)$. Further, since $x_k/x_{k-1} \le \rho < 1$, we have that $x_k/x_{k-m} \le \rho^m$ and hence

$$Q_{k-m,s}^{(k)} = \left[(1 + \rho^m)/(1 - \rho^m)\right] \cdot O\left(x_k^s\right) = O\left(x_k^s\right)$$

Therefore, the proof of Lemma (3.22) is complete.

Proof of Theorem (3.17). We first establish the following proposition which is stronger than (3.20). Under the hypothesis of Theorem (3.17).

$$P_{k-n}^{(k)} = a_0 + a_{n+1}\, Q_{k-n,n+1}^{(k)} + \cdots + a_m\, Q_{k-n,m}^{(k)} + O\left(x_k^{m+1}\right) \tag{3.26}$$

Proof is again by induction on n . For $n = 0$, the statement follows from (3.18) and the fact that $Q_{k,s}^{(k)} = x_k^s$. Assume statement (3.26) is true for the case $n-1$. Then

$$P_{k-n}^{(k)} = \left[x_k\, P_{k-n}^{(k-1)} - x_{k-n}\, P_{k-n+1}^{(k)}\right] \Big/ (x_k - x_{k-n})$$

and by the induction hypothesis, we have

$$P_{k-n}^{(k)} = \Big\{ x_k \Big[a_0 + a_n Q_{k-n,n}^{(k-1)} + \cdots + a_m Q_{k-n,m}^{(k-1)} + O\left(x_{k-1}^{m+1}\right) \Big]$$

$$- x_{k-n} \Big[a_0 + a_n Q_{k-n+1,n}^{(k)} + \cdots$$

$$+ a_m Q_{k-n+1,m}^{(k)} + O\left(x_k^{m+1}\right) \Big] \Big\} \Big/ (x_k - x_{k-n})$$

$$= a_0 + a_n Q_{k-n,n}^{(k)} + a_{n+1} Q_{k-n,n+1}^{(k)} + \cdots + a_m Q_{k-n,m}^{(k)}$$

$$+ \Big[(x_k / x_{k-n}) \, O\left(x_{k-1}^{m+1}\right) - O\left(x_k^{m+1}\right) \Big] \Big/ \Big((x_k / x_{k-n}) - 1 \Big)$$

Since $Q_{k-n,n}^{(k)} = 0$ by (3.23), and by the proof of (3.25), statement (3.26) is true. Finally, since

$$Q_{k-n,n+1}^{(n)} = (-1)^n x_{k-n} \cdots x_k$$

and

$$Q_{k-n,n+i}^{(k)} = O\left(x_k^{n+i}\right)$$

for $i = 2, \cdots, m-n$, (3.20) is true.

Finally, if $a_n \neq 0$, then

$$\left[P_{k-n}^{(k)} - a_0\right] \Big/ \left[P_{k-n+1}^{(k)} - a_0\right]$$

$$= \left[(-1)^n a_{n+1} x_{k-n} \cdots x_k + O\left(x_k^{n+2}\right)\right] \Big/$$

$$\left[(-1)^{n+1} a_n x_{k-n+1} \cdots x_k + O\left(x_k^{n+1}\right)\right]$$

$$= \left[-(a_{n+1}/a_n)\, x_{k-n} + O\left(x_k^2\right)\right] \Big/ \left(1 + O(x_k)\right)$$

$$= O(x_k)\ ,$$ which implies (3.21).

Therefore, if $a_n \neq 0$, the n^{th} column converges faster than the $(n-1)^{st}$ column.

This theorem is now applied to the general scheme developed in the Romberg Integration Section. Using the fact that the coefficients a_n occurring in the expansion of $T(h)$ in (3.16) have the form

$$\left[(B_{2n})/[(2n)\,!]\right]\left[f^{(2n-1)}(b) - f^{(2n-1)}(a)\right]$$

where the B_{2n} are the Bernoulli numbers, we have

(3.27) COROLLARY. If $f^{(2m+2)}(t)$ exists and is continuous for $a \le t \le b$, and if $0 < \sigma \le h_k/h_{k-1} \le \rho < 1$ for all k, then for $n < m$, the entries in the n^{th} column of (2.4) satisfy

$$T_{k-n}^{(k)} = \int_a^b f(t)\,dt$$

$$+ (-1)^n a_{n+1}(h_{k-n} \cdots h_k)^2 + O\left(h_k^{2n+4}\right) \text{ as } k \to \infty \tag{3.28}$$

Furthermore, if

$$f^{(2n-1)}(b) \ne f^{(2n-1)}(a) \tag{3.29}$$

the entries in the n^{th} column converge to $\int_a^b f(t)\,dt$ faster than those in the $(n-1)^{st}$ column.

If we further assume that f is analytic on $[a,b]$, then it follows from results of Gragg[8] and Bulirsch and Stoer[9] that

(3.30) THEOREM. If $T(h)$ has an asymptotic expansion in powers of h^2 (guaranteed if f is analytic on $[a,b]$), and if $0 < \sigma \le h_k/h_{k-1} \le \rho < 1$ for all k, then for each $m \ge 0$, constants E_m exist such that

$$\left|T_0^{(k)} - a_0\right| \le E_{m+1}(h_k \cdots h_{k+m})^2 \tag{3.31}$$

Hence, if (3.28) and (3.31) are true, and if $a_{m+1} \neq 0$, then the principal diagonal converges to a_0 faster than the m^{th} column of the array (2.4). Therefore, if $a_m \neq 0$ for all $m \geq 1$, then the principal diagonal converges to a_0 faster than any column of the array (2.4).

In ref. 1 it is noted that Corollary (3.27) suggests which functions may not work well with the scheme. For example, functions whose low-order derivatives do not exist at the end points of integration, would make the expression (3.29) for the corresponding low-order coefficients meaningless. Also, periodic functions whose odd-order derivatives are equal at a and b we might expect not to be adaptable to the scheme. On the other hand, functions which are analytic or have high-order derivatives on $[a,b]$, and are not periodic, we would expect to be, in many cases, particularly adaptable to this scheme.

Bauer, Rutishauser, and Stiefel[2] remark that the arguments used to prove Theorems (3.10) and (3.11) can be applied to the more general case if only $h_k/h_{k-1} \leq \rho < 1$ for all k. Further, it is noted in ref. 2 that Lemma (3.7) guarantees the numerical stability of the Romberg scheme, but for more slowly increasing sequences N_k, the susceptibility to round-off error is increased.

CONCLUDING REMARKS

As noted previously at the end of the Romberg Integration Section, it would seem practical to choose a sequence N_k less rapidly increasing than the sequence 2^k. One choice that would certainly minimize the number of calculations at each step would be $N_k = k + 1$, $k = 0,1,\cdots$. However, this choice obviously does not satisfy the requirement $h_k/h_{k-1} \le \rho < 1$ for all k and, as noted in ref. 2, can cause severe numerical instability if many columns of the table (2.4) are computed.

Another choice, suggested by Bulirsch[10] is

$$N_k = \begin{cases} 1 & , \quad k = 0 \\ 2^{(k+1)/2} & , \quad k \text{ odd} \\ 3 \cdot 2^{k/2-1} & , \quad k \text{ even} \end{cases}$$

That is, $N_k = 1,2,3,4,6,8,12,16,\cdots$. In this case $\rho = 3/4$.

Another choice suggested in ref. 2 is the sequence $N_k = 1,2,3,6,9,18,27,54,\cdots$ (all powers of 3 and their doubles). For this choice $h_k/h_{k-1} \le \rho < 1$ for all k,

but the modification is more susceptible to round-off errors than the Romberg scheme, since the sum $\sum_{i=0}^{m} |c_{m,m-i}|$ is higher than that for the Romberg method (up to 3.5).

The best choice of sequences appears to depend on the function, or at least class of functions, being integrated. In ref. 2 the function $1/x$ is integrated between 1 and 2 using the $1,2,3,6,9,\cdots$ modification. It is noted that even if no improvement on the Romberg scheme can be made, it does appear that computing time will be reduced to some degree in the long run.

There is a very extensive derivation and discussion of the Romberg algorithm and its generalizations in ref. 2. Bulirsch[10] has extended the method of Romberg to any sequence of numbers h_i with $\lim_{i\to\infty} h_i = 0$, by considering a linear matrix transformation of the sequence $T(h_i)$. Meir and Sharma[11] give an improvement of the result of Bulirsch. Stroud[12] has considered error estimates for the Romberg procedure, and compared them with error estimates of the Gaussian formulas. In a recent paper by Bulirsch and Stoer,[13] it is proposed to use a Romberg-like scheme based on rational function extrapolation. The authors give applications of their method in refs. 13 and 14, and compare

it with the Romberg scheme using polynomial interpolation in refs. 13 and 15.

The Romberg algorithm and its generalizations used for the numerical integration of definite integrals are based on the assumption that the trapezoidal approximation with step h has an asymptotic expansion in powers of h^2. It is proposed in refs. 2 and 9 to apply similar ideas to the solution of first-order ordinary initial-value problems using Euler's method as the basic discretization. The corresponding asymptotic expansion then also contains odd powers of h. Gragg[16] has established the existence of simple discretizations of both first and special second-order systems which have asymptotic expansions in powers of h^2. He then proposes to apply the modification of Bulirsch and Stoer to obtain the solution for this type of ordinary initial-value problem. Refs. 2 and 1 give examples where the basic assumption of the existence of an asymptotic expansion of $T(h)$ in powers of h^2 is not valid.

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